Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 109 °C

Global applicability domain: Inside

Local applicability domain index: 9.73e-01

Confidence level: 8.96e-01

Nearest Neighbors from the Training Set

Image not found
2,3,4-Trimethylpentane
Measured: 114
Predicted: 109

Image not found
Pentane, 2,3,3-trimethyl-
Measured: 115
Predicted: 109

Image not found
2,2,4-Trimethylpentane
Measured: 99.2
Predicted: 109

Image not found
(3S)-2,2,3-Trimethylpentane
Measured: 110
Predicted: 109

Image not found
Butane, 2,2,3,3-tetramethyl-
Measured: 106
Predicted: 108